Recent developments in (non-relativistic) mean-field theories

Michael Bender

IP2I Lyon, CNRS/IN2P3, Université Claude Bernard Lyon 1, Villeurbanne, France

Plenary meeting of the french low energy nuclear physics community

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A brief categorization of nuclear energy density functional methods

- Only presently available method that can be applied to describe numerous properties of and phenomena in even-even, odd, odd-odd nuclei within a universal framework using a universal parametererisation of the effective in-medium nucleon-nucleon interaction described in the form of an energy density functional that only depends on one-body density (matrices).
- "numerically simple" (diagonalisation of a one-body problem within a fixed-point iteration)
- achieved by working with densities provided by symmetry-breaking auxiliary states.

There are several levels of nuclear energy density functional (EDF) methods:

- Self-consistent mean-field models
  - "Hartree-Fock" (HF)
  - "Hartree-Fock-Bogoliubov" (HFB)
  - "nuclear Density Functional Theory" (nuclear DFT)
  - single-reference EDF methods

  Note: what is done by practitioners almost never complies with the rigorous definition of the concept of HF/HFB/DFT as found in textbooks.
- Time-dependent (TD) mean-field models (TDHF, THHFB), various extensions to make the outcome non-deterministic, . . .

"Beyond mean-field methods"

- (linear) response: linearisation of TDHF, (quasi-particle) random phase approximation ((Q)RPA) various diagrammatic extensions to include correlations, . . .
- Symmetry restoration (projection on particle number, angular momentum, parity,. . .)
- (non-orthogonal) configuration mixing, aka "Generator Coordinate Method" (GCM)

Phenomena that can be modeled with nuclear EDF methods

- (ground-state) binding energies and their differences
- excitation energies of shape isomers, collective rotational bands, one-quasiparticle energies, multi–quasiparticle energies, . . .
- nuclear (charge) density distributions and their moments, charge form factor, (charge) radii, deformations, electric multipole moments, Kumar shape invariants, magnetic multipole moments, . . .
- Fission barriers, dynamics lifetimes fragment distributions, . . .
- Large-amplitude collective motion, giant resonances, . . .

- mass spectroscopy
- electron scattering
- scattering with strongly-interacting probes
- laser spectroscopy
- γ-ray and conversion electron spectroscopy
- decay spectroscopy
- Coulomb excitation
- . . .

Black: specific states in specific nuclei can be models at the self-consistent mean-field level

Blue: with few exceptions requires a beyond-mean-field method

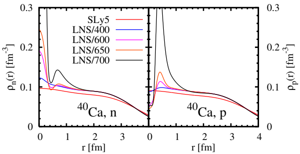
Ongoing efforts

Main directions of present efforts

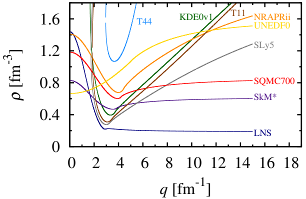
- Goal: larger set of phenomena that is simultanenously described by a given parameterisation of the EDF within a consistent numerical description.
- more general forms of the EDF
    - higher-order terms within existing forms such as Skyrme EDF (contact interaction with gradients; EDF built from local (spin) densities, currents, kinetic densities) Gogny force (Gaussian finite range force; EDF built from local and non-local (spin) densities) ...
    - different form altogether such as the Fayans EDF (EDF built from local (spin) densities) "regularized pseudo-potentials" (Gaussian finite range interaction with gradients), ...
- improved adjustment protocols of the parameter sets (estimates of statistical errors, analysis of correlations between observables and parameters, machine-learning assisted large-scale adjustment to thousands of data, ...)
- larger set of observables entering the adjustment protocols, either concerning properties of nuclei, or general features that (absence of unphysical instabilities, surface tension in semi-infinite matter pairing properties in infinite matter, ...
- codes that can efficiently and handle more general forms of the EDF, more complex shapes and more complex situations for the orientation of angular momenta relative to the shape)

Finite-size instabilities in the $S = 0$, $T = 1$ channel:

T. Lesinski, K. Bennaceur, T. Duguet, J. Meyer, PRC 74, 044315 (2006)



Lesinski, Bennaceur, Duguet, Meyer, PRC C74 (2006) 044315



Hellemans, Pastore, Duguet, Bennaceur, Davesne, Meyer, Bender, Heenen, PRC 88 (2013) 064323

Note: instability in the $S = T = 0$ channel is physical. Similar instabilities found in $S = 1$ channels. Can emerge for contact and finite-range interaction, relativistic and non-relativistic ones.

Pairing needs readjustment for each value of m^* / m

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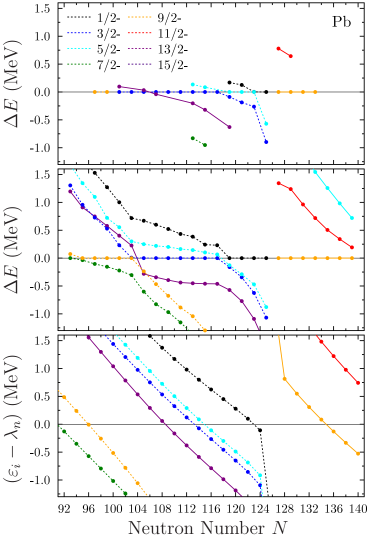
Problem: imperfect single-particle spectra



Bender (et al?) (to be published)

Pairing needs readjustment for each value of m^*/m
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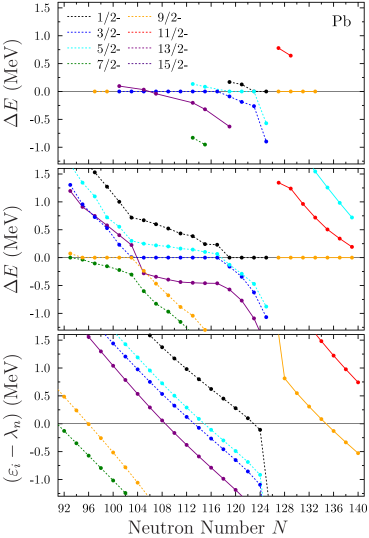
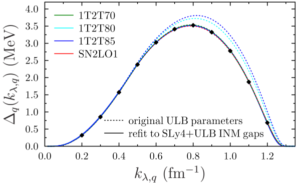
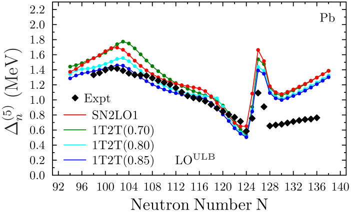
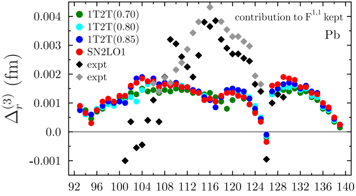


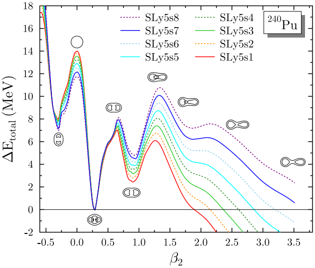




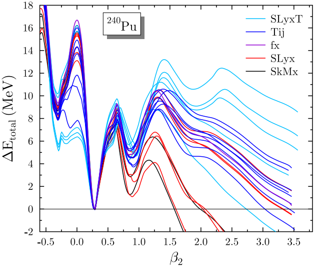


Bender (et al?) (to be published)

parameter sets with systematically varied a_{surf}

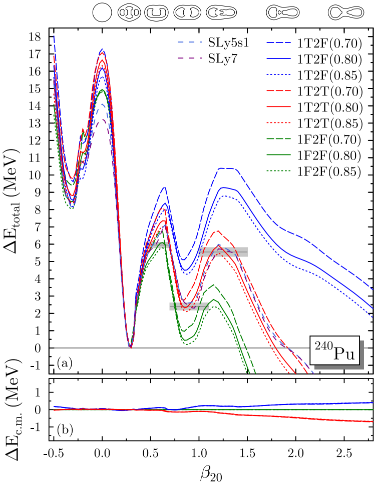


existing parameter sets (mostly from Lyon)



Jodon, Bender, Bennaceur, Meyer, PRC 94 (2016) 024335

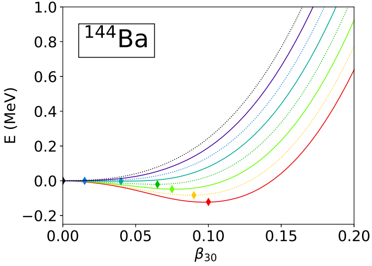
Role of centre-off-mass correction



Da Costa, Bennaceur, Meyer, Ryssens, Bender, PRC 109 (2024) 034316 ;
see also Bender, Rutz, Reinhard, Maruhn, EPJ A7 (2000) 467

Octupole deformation of ^{144}Ba:

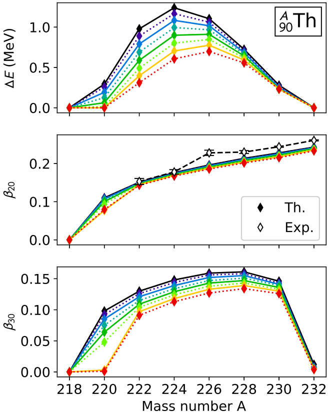
red: SLy5s1 ($a_{\mathrm{surf}} = 17.55$ MeV)
purple: SLy5s8 ($a_{\mathrm{surf}} = 18.89$ MeV)



Relevant for finding “exotic” ground-state shapes!

Octupole deformation of Th isotopes:

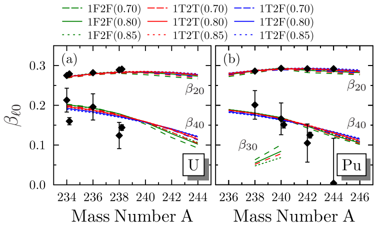
inverted colour code:
purple: SLy5s1 ($a_{\mathrm{surf}} = 17.55$ MeV)
red: SLy5s8 ($a_{\mathrm{surf}} = 18.89$ MeV)



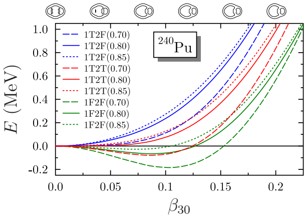
Ryssens, Bender, Bennaceur, Heenen, Meyer, PRC 99 (2019) 044315

Control of surface energy: relevance for exotic shape phenomena

Ground-state deformation of actinides

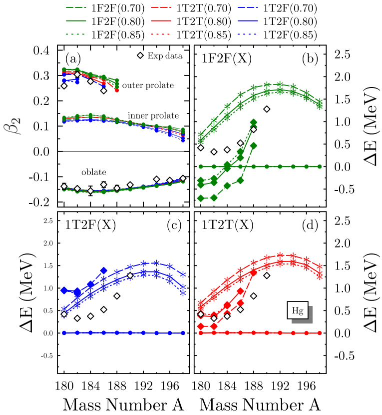


Octupole softness of ^{240}Pu



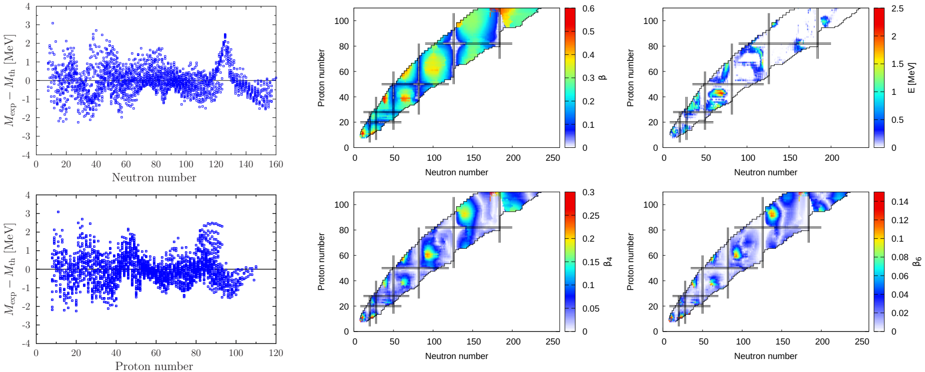
Da Costa, Bennaceur, Meyer, Ryssens, Bender, PRC 109 (2024) 034316

Shape coexistence in Hg



Note: the minima are generated by shell effects, but the energy difference between minima and the stiffness of the deformation energy around the minima is controlled by the surface energy.

Large-scale mass fits: BSkGx ("Brussels Skyrme on a Grid")



BSkG1: σ of 2457 masses = 0.734 MeV (and lower for mass differences), σ of 884 chare radii = 0.0239 fm

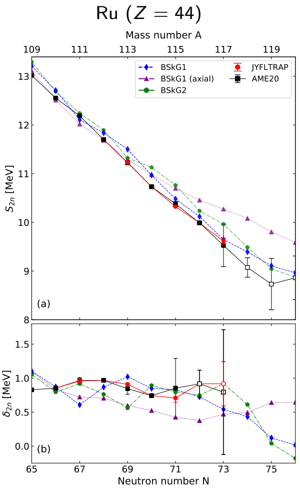
Scamps, Goriely, Olsen, Bender, Ryssens, EPJ A 57 (2021) 333

BSkG2: full blocking for odd- and odd-odd nuclei with time-odd contributions, adjustment of fission barriers and excitation energies of superdeformed isomers. σ of 2457 masses = 0.668 MeV (and lower for mass differences), σ of 884 charge radii = 0.0274 fm, σ of 45 primary barriers = 0.44 MeV, σ of 45 secondary barriers = 0.47 MeV, σ of 28 fission isomers = 0.49 MeV.

Ryssens, Scamps, Goriely, Bender, EPJ A 58 (2022) 246

BSkG3, BSkG4: additional density-dependent terms, generalised pairing EDF.

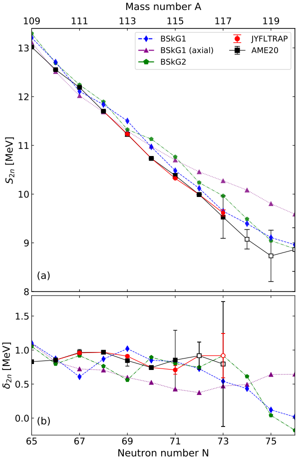
BSkG5: higher-order gradient terms instead of additional density-dependent terms.



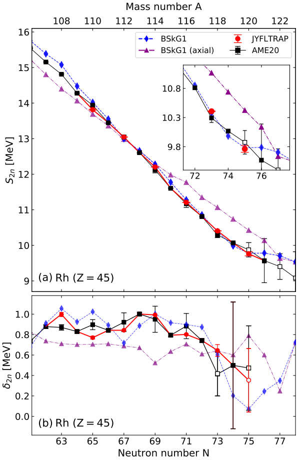
Hukkanen et al, PRC 108 (2023) 064315

Masses in the Zr-Mo-Ru-Rh-Pd region

Ru ($Z = 44$)



Rh ($Z = 45$)



Hukkanen et al, PRC 108 (2023) 064315

Hukkanen et al, PRC 107 (2023) 014306

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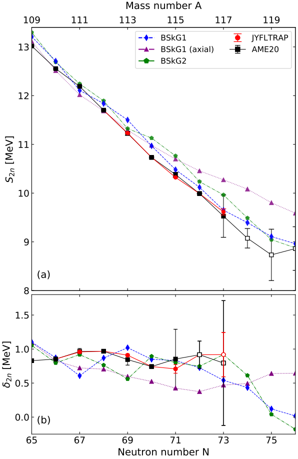
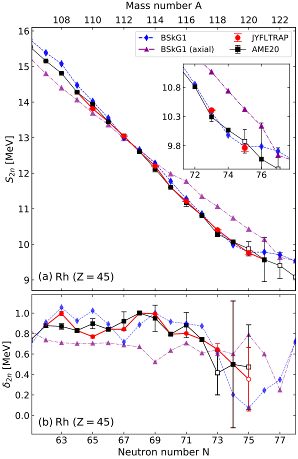


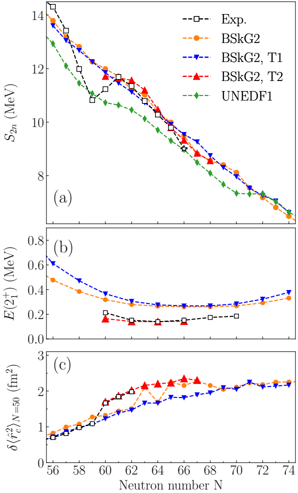
Hukkanen et al, PRC 108 (2023) 064315

Rh ($Z = 45$)

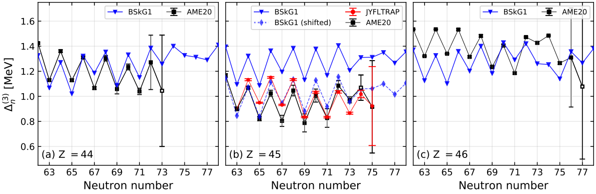


Hukkanen et al, PRC 107 (2023) 014306

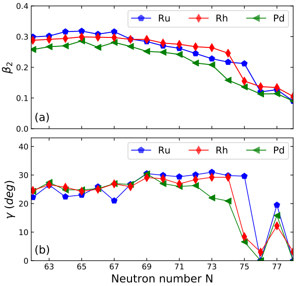
Zr ($Z = 40$)



Hukkanen et al, PLB 856 (2024) 138916

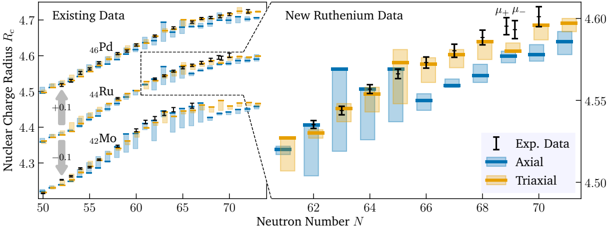


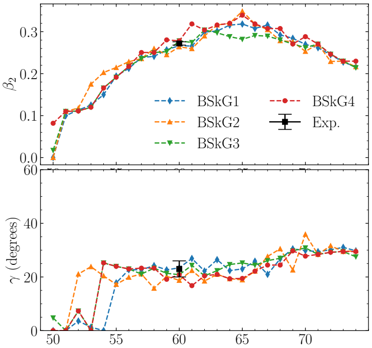
Systematic effect missing in the odd-even staggering of neutron gap of odd-Z isotopes: p-n residual interaction of 250 keV in odd-odd nuclei?

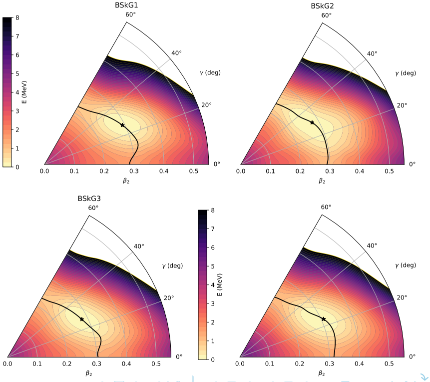


Hukkanen et al, PRC 107 (2023) 014306

A further paper casts a shadow of doubt on the attribution of quantum numbers to the ground and isomeric state of ^{114}Rh Stryjczyk et al, PLB 862 (2025) 139359

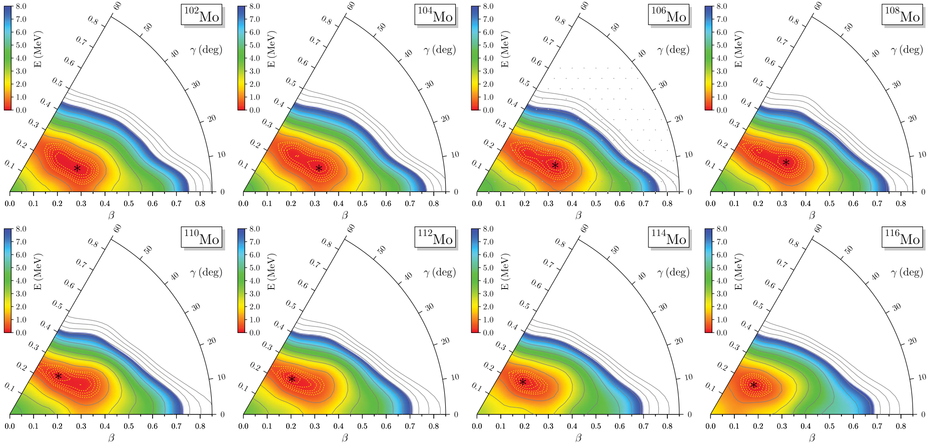






Maass et al, accepted for PRL.

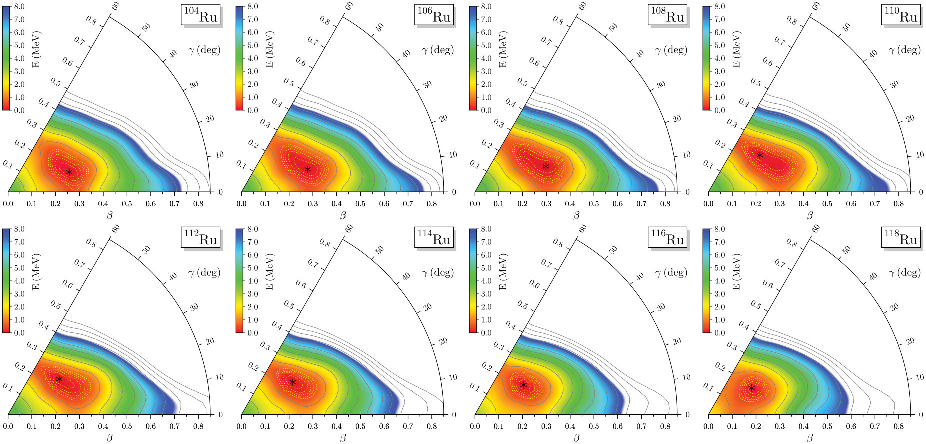
Deformation energy surfaces of Mo isotopes obtained with BSkG2



- The position of the minimum is indicated by a black asterisk.
- Solid iso-energy lines in grey are 1 MeV apart staring with the energy of the global minimum.
- To better see the fine structure of the energy surfaces around the minima, the dotted isolines in yellow indicate 0.1, 0.2, 0.3, 0.4 and 0.5 MeV above the ground state.

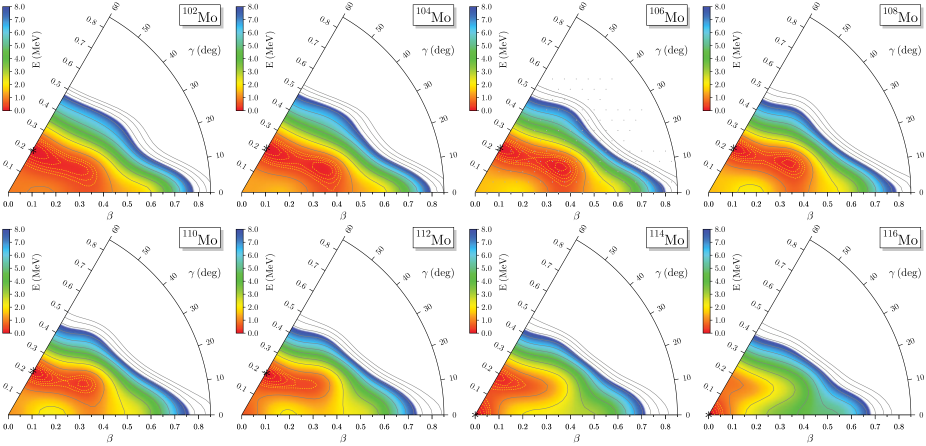
Bonatsos et al, submitted to PRC

Deformation energy surfaces of Ru isotopes obtained with BSkG2



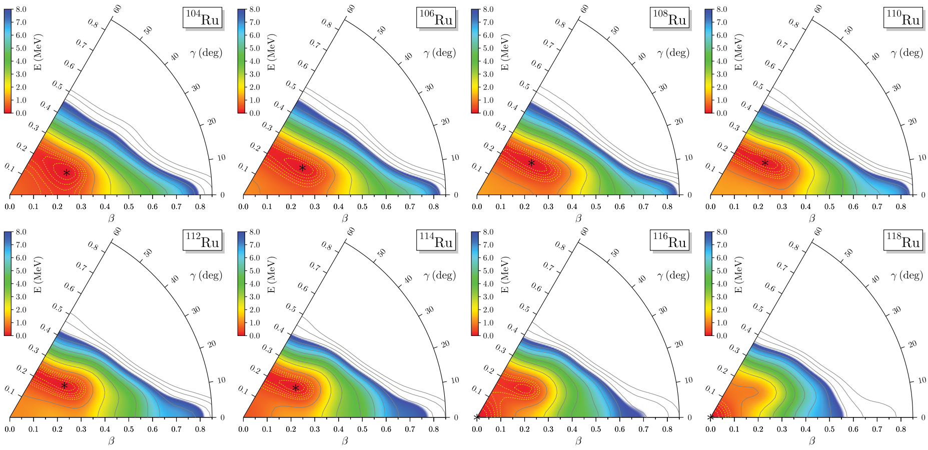
Bonatsos et al, submitted to PRC

Deformation energy surfaces of Mo isotopes obtained with SLy7* (1T2T(0.80))



Bonatsos et al, submitted to PRC

Deformation energy surfaces of Ru isotopes obtained with SLy7* (1T2T(0.80))



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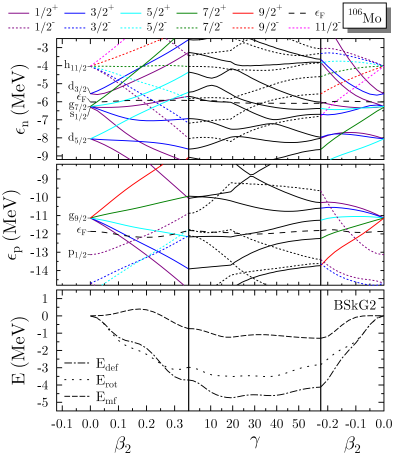
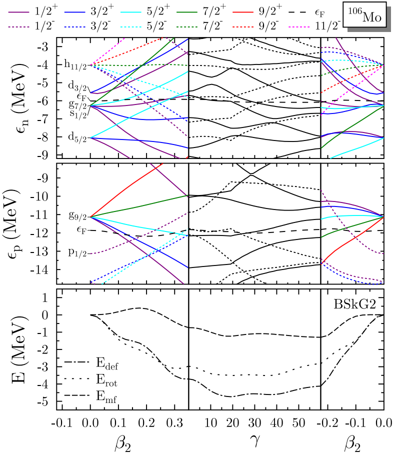
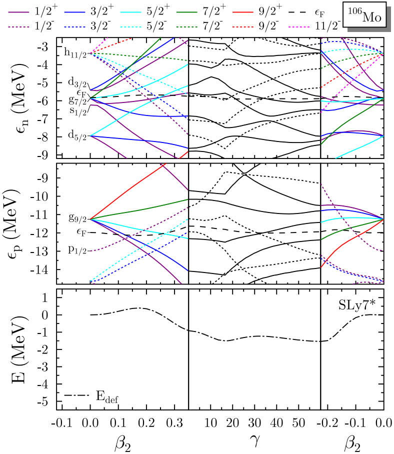


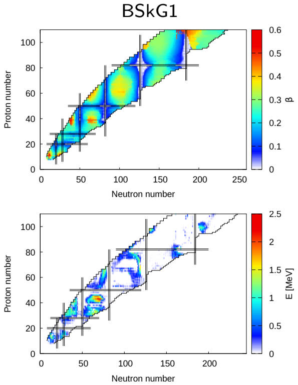
Deformation energy surfaces of Ru isotopes obtained with SLy7* (1T2T(0.80))



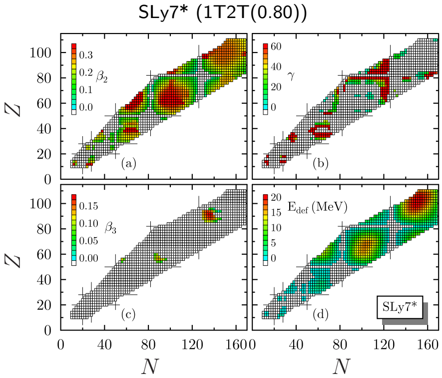


Bonatsos et al, submitted to PRC

Deformation energy surfaces of Ru isotopes



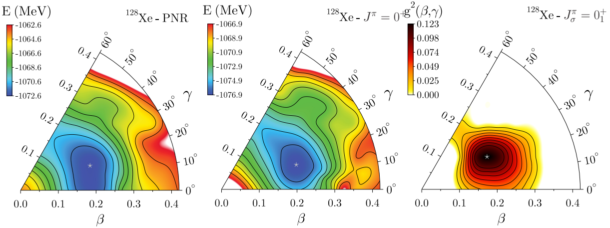
Scamps, Goriely, Olsen, Bender, Ryssens, EPJ A 57 (2021) 333



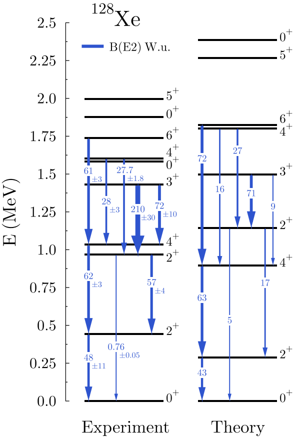
Bender (to be published)

- Triaxial nuclei are those in any colour on the lower panel for BSkG1 and those indicated in green on the panel indicating for γ for SLy7* (1T2T(0.80)).
- The rotational correction of the BSkGx drives nuclei towards triaxial shapes.

Beyond-mean-field description of triaxial nuclei (with SLyMR1): ^{128}Xe

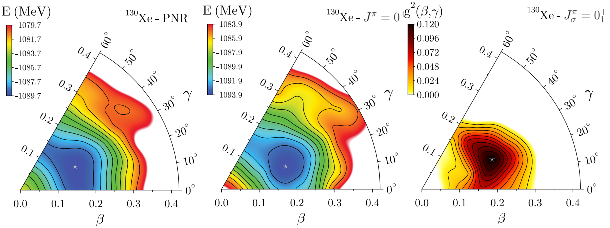


Quantity	Experiment	Theory
$E(0_1^+)$	-1080.743	-1077.956
$r_{\text{rms}}(0_1^+)$	4.7774(50)	4.738
$\mu(2_1^+)$	$+0.68(7)$	$+0.6$
$\mu(4_1^+)$		$+1.2$
$\mu(2_2^+)$		$+0.6$
$Q_s(2_1^+)$		-0.8
$Q_s(4_1^+)$		-0.9
$Q_s(2_2^+)$		$+0.8$
$B(E2: 2_1^+ \to 0_1^+)$	1839(421)	1664

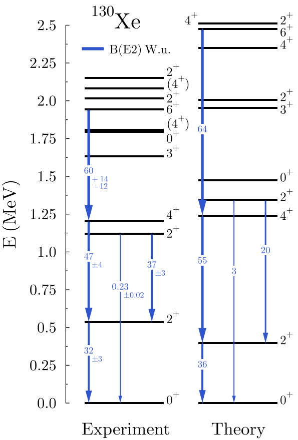


Bally, Giacalone, Bender, EPJA 58 (2022) 187

Beyond-mean-field description of triaxial nuclei (with SLyMR1): ^{130}Xe

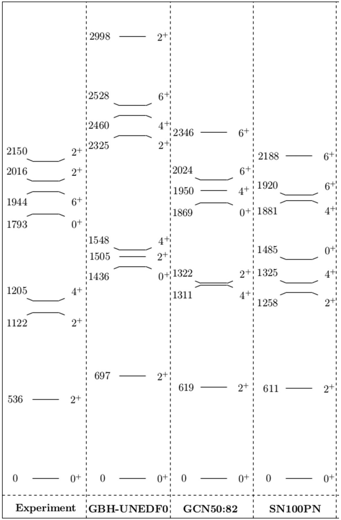


Quantity	Experiment	Theory
$E(0_1^+)$	-1096.905	-1095.058
$r_{\rm rms}(0_1^+)$	4.7818(49)	4.741
$\mu(2_1^+)$	+0.67(10)	+0.6
$\mu(4_1^+)$	+1.7(4)	+1.3
$\mu(2_2^+)$	+0.9(2)	+0.6
$Q_s(2_1^+)$	-0.38(+17,-14)	-0.7
$Q_s(4_1^+)$	-0.41(12)	-0.7
$Q_s(2_2^+)$	+0.1(1)	+0.6
$B(E2 : 2_1^+ \to 0_1^+)$	1252(117)	1416

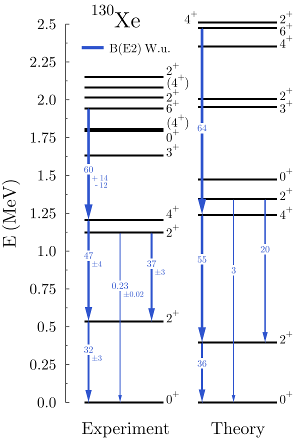


Bally, Giacalone, Bender, EPJA 58 (2022) 187

Beyond-mean-field description of triaxial nuclei (with SLyMR1): ^{130}Xe



Morrison et al, PRC 102 (2020) 054304

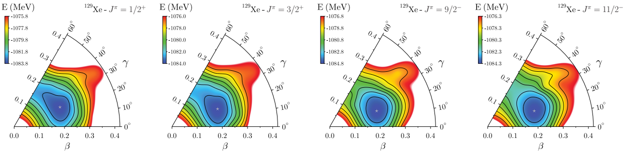


Bally, Giacalone, Bender, EPJA 58 (2022) 187

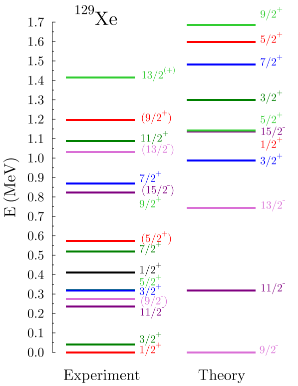
Quantity	Theory	Experiment
β_r	0.18	0.17(1)
γ_d	21°	28°
β_c	0.19	n.a.
$\Delta\beta_c$	0.04	n.a.
γ_c	23°	n.a.
$\Delta\gamma_c$	16°	n.a.
β_k	0.16	0.17(2)
$\Delta\beta_k$	0.02	
γ_k	28°	23(5)°
$\Delta\gamma_k$	12°	

Bally, Giacalone, Bender, EPJA 58 (2022) 187

- β_r, γ_d: rigid-rotor Davydov model Davydov et al, NP 8 (1958) 237
- β_c, γ_c: average intrinsic deformation of the GCM state and its standard deviation
- β_k, γ_k, $\Delta\beta_k$, $\Delta\gamma_k$: Kumar invariants from sums over $E2$ matrix elements
- Experimental values for Kumar invariants from Morrison et al, PRC 102 (2020) 054304



Quantity	Experiment	Theory
$E(1/2^+_1)$	-1087.649	-1084.720
$r_{\text{rms}}(1/2^+_1)$	4.7775(50)	4.736
$\mu(1/2^+_1)$	-0.78	-0.2
$\mu(3/2^+_1)$	+0.58(8)	+1.2
$\mu(3/2^+_2)$		-0.1
$\mu(11/2^-_1)$	-0.89	-1.1
$Q_s(3/2^+_1)$	-0.39(1)	+0.4
$Q_s(3/2^+_2)$		-0.4
$Q_s(11/2^-_1)$	+0.63(2)	+0.8



- moments of the intruder state are reasonably well described
- moments of normal-parity states are not really well described
- energetic order of states is incorrect

Bally, Giacalone, Bender, EPJA 58 (2022) 187

Charge radii of Fm and No isotopes

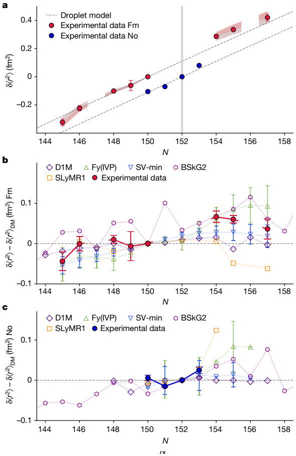


Fig. 2 | Comparison of experimental mean-square charge radii data with different nuclear model predictions. a, Experimental results of $\delta\langle r^2\rangle$ of fermium isotopes as a function of N relative to ^{250}Fm (red) and of nobelium isotopes relative to ^{254}No (blue). The error bars show statistical uncertainties (one standard deviation) and the red shaded bands represent systematic uncertainties in the prediction of the atomic parameters (Methods). The observed smooth trend along the isotopic chain is independent of the atomic parameters as their uncertainty is only of a systematic nature, thus affecting all extracted $\delta\langle r^2\rangle$ in the same manner. Predictions of the spherical droplet model are shown with dashed lines for comparison with the experimental data. **b**,**c**, $\delta\langle r^2\rangle$ for fermium (**b**) and nobelium (**c**) predicted by five theoretical models relative to the droplet-model (DM) reference. Experimental data (red and blue solid symbols) are compared with predictions of different models.

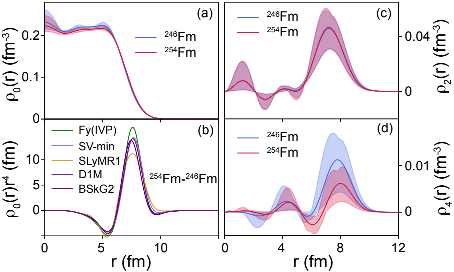
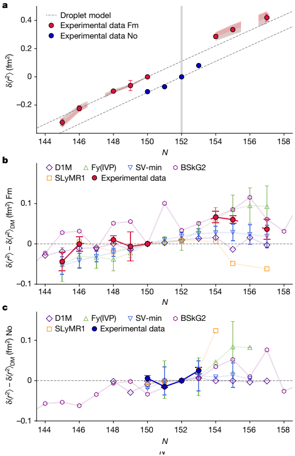


Fig. 3 | Comparison of different model predictions for multipole proton radial densities of ^{246}Fm and ^{254}Fm. a–d, Monopole radial densities (**a**), r^4-weighted difference between monopole radial densities of ^{254}Fm and ^{246}Fm (**b**), quadrupole radial densities (**c**) and hexadecapole radial densities (**d**). The maximum range of model predictions is marked by bands in **a**, **c** and **d**; the solid lines represent the average of the models.

Warbinek et al, Nature 634 (2024) 1075



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Une étude expérimentale indique que tous les isotopes de noyaux superlourds pourraient bien être déformés

14 avril 2025

RÉSULTATS SCIENTIFIQUES PHYSIQUE NUCLÉAIRE

L'étude conduite sur 8 isotopes du fermium par une collaboration impliquant des scientifiques du GANIL montre que la forme des noyaux superlourds semble échapper à la règle observée chez les noyaux plus légers. Ces derniers peuvent en effet changer de forme de façon très abrupte dès que leurs couches de nucléons ne sont pas entièrement remplies. Or, les différents isotopes de Fermium observés par la collaboration grossissent tranquillement avec le nombre de neutrons, quel que soit le taux de remplissage des couches de nucléons, comme si les effets quantiques dus aux fermetures de couches étaient effacés. Ce résultat expérimental, en accord avec les prédictions de certains modèles de physique nucléaire, laisse penser que la règle pourrait bien s'appliquer à l'ensemble des noyaux super-lourds.

text discretely replaced on the IN2P3's website since this screenshot was taken in may 2025

- Large-scale symmetry-breaking calculations of the entire nuclear chart . . .
- . . . including odd and odd-odd nuclei
- Better controlled surface energy improves description of exotic shape degrees of freedom and fission barriers.

Outlook:

- extended forms of the functional for better control of single-particle streucture . . .
- . . . in a form that can be safely handled in beyond-mean-field calculations?

People involved in the recent theoretical and numerical developments . . .

Benjamin Bally	CEA Saclay, now TU Darmstadty
Wouter Ryssens	Université Libre de Bruxelles
Jacques Meyer	IPN Lyon
Karim Bennaceur	IP2I Lyon
Robin Jodon	IP2I Lyon
Philippe da Costa	IP2I Lyon
Valentin Guillon	IP2I Lyon

Many thanks also to everybody involved in the analysis of these results, in particular to the experimentalists who invited us to participate in the interpretation of their new data!